Integration of BOUT++ numerical framework into IFERC-CSC

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Abstract

RECENTLY the open source BOUT++ code [1] has been deployed on IFERC-CSC [2] Helios super computer in Rokkasho. This code is applied to simulate L/H transition in JT-60SA plasmas, which will be compared with results obtained by an integrated transport simulation [3]. Then, ITB formation and ELM crush, which occur subsequently, will be investigated. We report on the present status of development within our lab. A new python toolset has been developed that allows for processing of EFIT experiment reconstructions in order to produce the necessary input files. A scaling experiment compares well with that of a Cray machine in USA. A number of benchmarks validates and verifies the code on Helios. An outline of future development is also presented.

1. Framework

THE BOUT++ framework, developed by Lawrence Livermore National Laboratory (LLNL), University of York (UK) and various partners around the world, provides a unified and modular solution for testing and analyzing plasma physics models investigating elms and pedestal dynamics. The code is written in C++ and uses finite differences, a variety of numerical methods and time integration solvers to advance a wide variety of equations. Main dependencies include NetCDF, FFTW and MPI. A number of optional solvers, such as PETSc, can be incorporated if needed. Primary advantages of the framework include

- Separating the numerical implementation from the physical algorithm allowing the user to focus on the formulation of the physics scheme.
- Utilizing a versatile 3D curvilinear coordinate system that can be easily adjusted to a given metric in a way that enhances accuracy and efficiency with a notable constrain that the field must be axisymmetric in the z coordinate.
- Able to handle nonlinear simulations and the diverter region.

2. Workflow

THE necessary input file can be constructed from any geqdsk/efit file computed by equilibrium codes or experimental reconstructions. A new toolset written in Python has been developed in Rokkasho, based on a corresponding one in IDL, that can create an input grid file for BOUT++ simulations. The aim was to take advantage of the advanced graphics capabilities of matplotlib libraries [4] and the mathematical prowess of python. During this preprocessing phase the equilibrium can be analyzed and integrated to produce an appropriate grid describing the initial conditions. In Fig.1 a JT60 profile is presented, as analyzed by the python routines, depicting the X and O points and a reference flux line (in blue).

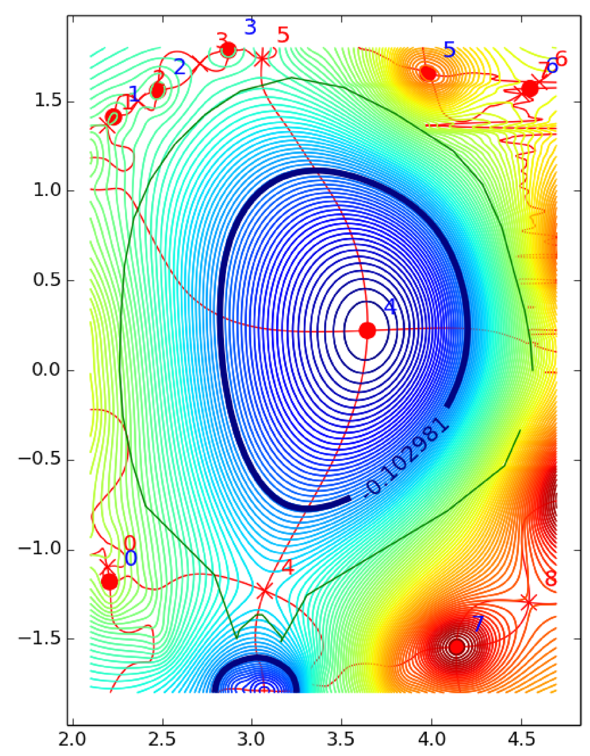
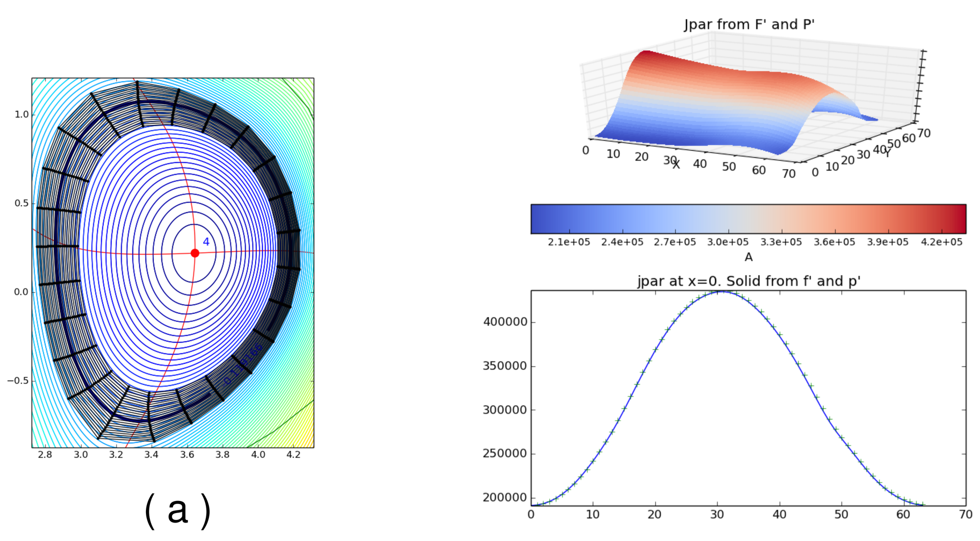


Figure 1: *Analysis of a JT60 equilibrium*

Based on this analysis a grid can be created (Fig.2(a)) and processed in order to assess its quality. Force balance can be enforced by independently adjusting pressure, toroidal field and poloidal arc-length while new quantities can be computed such as the parallel current profile (Fig.2(b)).



(a) (b)

Figure 2: *Generated grid for use with BOUT++ (a) and computed $J_{||}$ (b).*

3. Post-Processing

A NUMBER of python scripts have been developed for analyzing the results based on matplotlib and Mayavi [5] libraries. These include computing radial mode structure, 3D visualization of poloidal filaments (Fig.3) and surface averaged radial profiles of the computed variables.

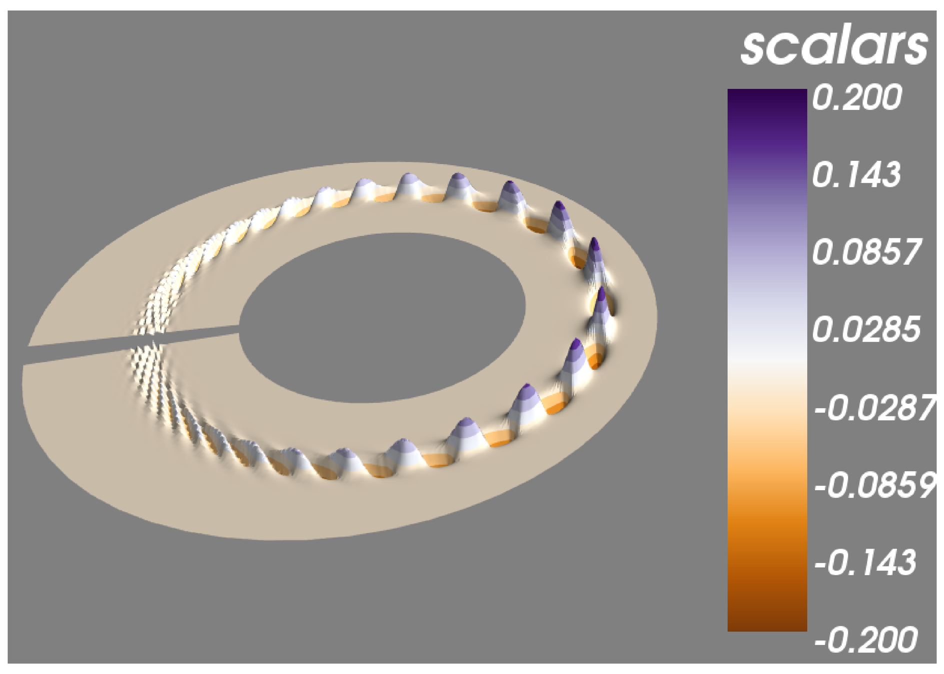
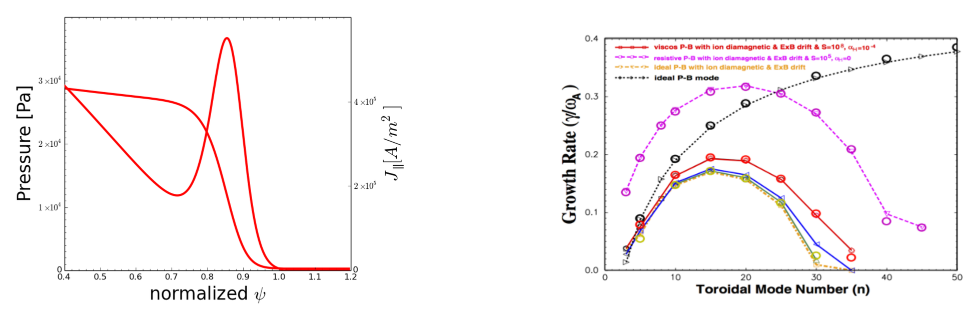


Figure 3: *3-D representation of filaments using Mayavi*

4. Validation

AS part of a benchmarking procedure, a number of results pertaining to peeling-ballooning stability were reproduced in order to check our installation and to provide an insight into the configuration settings. The pedestal profiles shown in Fig.4(a) were used as input and the comparison with data presented in [6] for the peeling-ballooning mode, which is attributed to type-I ELMs, is given in Fig.4(b).



(a) (b)

Figure 4: *Initial profiles (a) and comparison of our results (open circles) with reported results (b).*

FURTHERMORE, a scaling experiment (Fig.5) was performed on Helios. Comparison with results from Hopper, a Cray computer in National Energy Research Scientific Computing Center in USA, suggests that the efficiency of our computational resources is on par. This also served as a verification of the MPI implementation of the code in Rokkasho.

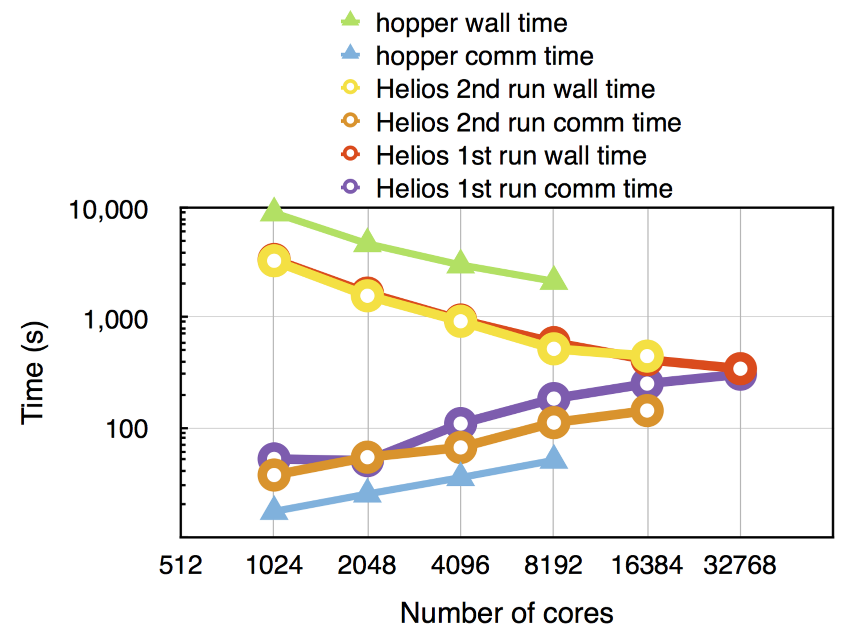


Figure 5: *Performance of BOUT++ on Helios and comparison with Hopper.*

5. Research program

A CHARACTERISTIC nonlinear set of equations solved with BOUT++ is based on the 3-field approximation evolving pressure P, vorticity U and magnetic potential ψ and can be formulated as

$$
\begin{aligned}
\rho_0 \frac{\partial U_1}{\partial t} &= -\frac{\rho_0}{B_0}\vec{b}_0 \times \nabla\phi_1 \cdot \nabla U_1 \\
&+ B_0^2 \left[\vec{b}_0 \cdot \nabla \left(\frac{J_{||1}}{B_0}\right) - \vec{b}_0 \times \nabla\psi_1 \cdot \nabla \left(\frac{J_{||0}+J_{||1}}{B_0}\right)\right] \\
&+ 2\vec{b} \times \vec{\kappa} \cdot \nabla P_1 \\
\frac{\partial \psi_1}{\partial t} &= -\frac{1}{B_0}\vec{b}_0 \cdot \nabla\phi_1 \\
\frac{\partial P_1}{\partial t} &= -\frac{1}{B_0}\vec{b}_0 \times \nabla\phi_1 \cdot \nabla (P_0 + P_1) \\
U_1 &= \frac{1}{B_0}\nabla_\perp^2 \phi_1 \\
J_{||1} &= -\frac{1}{\mu_0} B_0 \nabla_\perp^2 \psi_1
\end{aligned}
$$

Introducing an appropriate heating component will lead to a pedestal formation allowing a complete simulation of the dynamics from L profile to H profile to ELM disruptions within the same computational framework. This way, recent integrated simulations [3, 7] can be revisited from first principles. Of particular interest is the area around the divertor (Fig.6). Preliminary results from BOUT++ suggest that the reported transport dynamics (Fig.7a,b) can be investigated, including pedestal formation (Fig.7c) and collapse (Fig.7d). The formulation and analysis of such a scheme is underway.

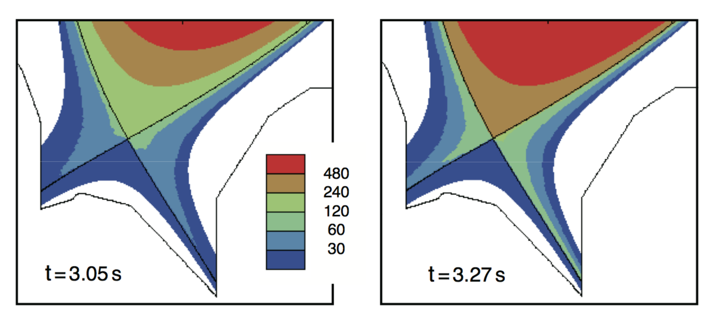


Figure 6: *2D contours of electron temperature (eV) in the R,Z plane before (left) and after (right) the L/H transition. Results reported in [3].*

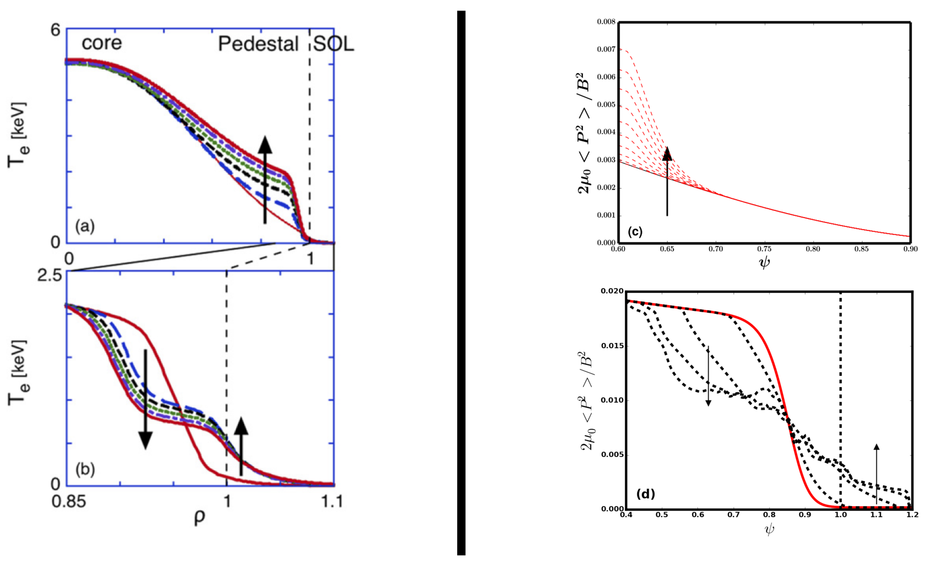


Figure 7: *Integrated simulations results before (a) and during an ELM event (b). BOUT++ results of pressure pedestal formation c) and collapse d).*

References

[1] https://bout.llnl.gov/ [2] http://www.iferc.org/ [3] M. Yagi *et al.*, *Contrib. Plasma Phys.*, **52**, 372 (2012). [4] http://matplotlib.org/ [5] Enthought, Inc, Mayavi project, http://code.enthought.com/projects/mayavi/. [6] B. X. Q. Xu *et al.*, *PRL* **105**, 175005 (2010). [7] N. Hayashi *et al.*, *Nucl. Fusion* **47** 682 (2007).